

LA-UR-19-28507

Approved for public release; distribution is unlimited.

Title: (U) Transport Corrections Implemented in SENSMSG

Author(s): Favorite, Jeffrey A.

Intended for: Report

Issued: 2020-09-25 (rev.1)

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Los Alamos

NATIONAL LABORATORY

memorandum

X-Computational Physics Division
Radiation Transport Applications Group
Group XCP-7, MS F663
Los Alamos, New Mexico 87545
505/667-1920

To/MS: Distribution
From/MS: Jeffrey A. Favorite / XCP-3, MS F663
Phone/Email: 7-7941 / fave@lanl.gov
Symbol: XCP-7:20-029(U) (LA-UR-19-28507)
Date: September 22, 2020 (Rev. 1)
August 20, 2019 (Rev. 0)

SUBJECT: (U) Transport Corrections Implemented in SENSMG

I. Introduction

Truncating the spherical harmonics expansion of the neutron scattering source in the Boltzmann transport equation leads to truncation error. Methods for approximately correcting for this truncation error are called *transport corrections*. The PARTISN multigroup discrete ordinates neutron transport code¹ has three transport correction options. These options can be specified in the SENSMG multigroup neutron sensitivity code^{2,3} and passed to PARTISN for the neutron transport.

SENSMG has now been updated to include exactly the effect of transport corrections on the computed sensitivities. Previously, SENSMG results were inconsistent with the transport solutions when transport corrections were used.

This report discusses the issues associated with computing sensitivities when transport corrections are used. A discussion of energy group-collapsing in the Nuclear Data Interface (NDI) is included because SENSMG now has to deal with that.

Section II of this report presents the transport corrections available in PARTISN. Section III discusses the calculation of sensitivities using transport-corrected cross sections. Section IV discusses the implementation of the equations of Sec. III into SENSMG. Section V presents results of an analytic test problem, and Sec. VI presents results of a realistic (nonanalytic) test problem. Section VII is a summary. The SENSMG input files for the test problems are listed in the appendix.

II. Transport Corrections

In PARTISN, the user inputs the desired transport correction using keyword `trcor` in block 5. In SENSMG, the user inputs the desired transport correction using keyword `-trcor` on the command line. The available options are the same: `no`, `diag`, `bhs`, and `cesaro`. The discussion in this section is a summary of the relevant section of Chapter 3 of the PARTISN manual.¹

The default is to apply no transport correction. This is also obtained with `trcor = no`.

The *diagonal* transport correction (`trcor = diag`) corrects the total and self-scattering cross sections using

$$\tilde{\Sigma}_t^g = \Sigma_t^g - \Sigma_{s, \text{ISCT}+1}^{g \rightarrow g}, g = 1, \dots, G \quad (1)$$

and

$$\tilde{\Sigma}_{s,l}^{g \rightarrow g} = \Sigma_{s,l}^{g \rightarrow g} - \Sigma_{s, \text{ISCT}+1}^{g \rightarrow g}, g = 1, \dots, G, l = 0, 1, \dots, \text{ISCT}, \quad (2)$$

where G is the number of energy groups (a user input), ISCT is the scattering expansion order (a user input), and the tilde represents the transport-corrected cross section.

The *Bell-Hansen-Sandmeier (BHS)* transport correction⁴ (`trcor = bhs`) corrects the total and self-scattering cross sections using

$$\tilde{\Sigma}_t^g = \Sigma_t^g - \sum_{g'=1}^G \Sigma_{s, \text{ISCT}+1}^{g \rightarrow g'}, g = 1, \dots, G \quad (3)$$

and

$$\tilde{\Sigma}_{s,l}^{g \rightarrow g} = \Sigma_{s,l}^{g \rightarrow g} - \sum_{g'=1}^G \Sigma_{s, \text{ISCT}+1}^{g \rightarrow g'}, g = 1, \dots, G, l = 0, 1, \dots, \text{ISCT}. \quad (4)$$

The *n'th-Cesàro-mean-of-order-2* transport correction (`trcor = cesaro`) corrects the scattering cross sections using

$$\tilde{\Sigma}_{s,l}^{g \rightarrow g'} = \frac{(\text{ISCT} + 2 - l)(\text{ISCT} + 1 - l)}{(\text{ISCT} + 2)(\text{ISCT} + 1)} \Sigma_{s,l}^{g \rightarrow g'}, g = 1, \dots, G, g' = 1, \dots, G, l = 1, \dots, \text{ISCT}. \quad (5)$$

These modified scattering cross sections do not affect the total cross section. It should here be noted that the Cesàro transport correction is not recommended.

PARTISN applies the transport correction to the macroscopic material cross sections. The output cross section file `macrxs` contains uncorrected cross sections. However, the cross sections output to the standard output file using `xsectp > 0` in block 5 are transport-corrected.

III. Transport-Corrected Sensitivities

The relative sensitivity $S_{R,\sigma_{t,i}}^g$ of a response R to the total cross section $\sigma_{t,i}^g$ of isotope i in energy group g is

$$S_{R,\sigma_{t,i}}^g = -\int_V dV \int_{4\pi} d\hat{\Omega} \Gamma^{*g}(r, \hat{\Omega}) N_i \sigma_{t,i}^g \psi^g(r, \hat{\Omega}), \quad (6)$$

where $\psi^g(r, \hat{\Omega})$ and $\Gamma^{*g}(r, \hat{\Omega})$ are the forward and adjoint angular fluxes, respectively, and N_i is the number density of isotope i in the material. The right side of Eq. (6) may have a denominator, depending on the response. The relative sensitivity $S_{R,\sigma_{s,l,i}}^{g \rightarrow g'}$ of R to the scattering cross section $\sigma_{s,l,i}^{g \rightarrow g'}$ of isotope i for expansion order l from energy group g to g' is

$$S_{R,\sigma_{s,l,i}}^{g \rightarrow g'} = \int_V dV \Gamma_l^{*g'}(r) N_i (2l+1) \sigma_{s,l,i}^{g \rightarrow g'} \phi_l^g(r) - \delta_{l0} \int_V dV \int_{4\pi} d\hat{\Omega} \Gamma^{*g}(r, \hat{\Omega}) N_i \sigma_{s,0,i}^{g \rightarrow g'} \psi^g(r, \hat{\Omega}), \quad (7)$$

where δ_{pq} is the Kronecker delta function and $\phi_l^g(r)$ and $\Gamma_l^{*g'}(r)$ are the forward and adjoint flux moments of order l . The second term on the right side appears because the isotropic scattering cross sections are included in the total cross section $\sigma_{t,i}^g$.

The relative sensitivity S_{R,N_i}^g in group g of R to the density of isotope i is

$$S_{R,N_i}^g = S_{R,\nu_i}^g + S_{R,\sigma_{t,i}}^g + S_{R,\sigma_{s,i}}^g, \quad (8)$$

where the relative sensitivity to total scattering out of group g is

$$S_{R,\sigma_{s,i}}^g = \sum_{l=0}^L \int_V dV \sum_{g'=1}^G \Gamma_l^{*g'}(r) N_i (2l+1) \sigma_{s,l,i}^{g \rightarrow g'} \phi_l^g(r). \quad (9)$$

S_{R,ν_i}^g is the contribution from the fission terms and is not discussed further in this report; see Ref. 3.

From Eqs. (3) and (4), when BHS transport correction is used, the relative sensitivity $S_{R,\sigma_{s,\text{ISCT}+1,i}}^{g \rightarrow g'}$ of R to the scattering cross section $\sigma_{s,\text{ISCT}+1,i}^{g \rightarrow g'}$ of isotope i for expansion order ISCT+1 from energy group g to g' is

$$S_{R,\sigma_{s,\text{ISCT}+1,i}}^{g \rightarrow g'} = -\sum_{l=0}^L \int_V dV \Gamma_l^{*g}(r) N_i (2l+1) \sigma_{s,\text{ISCT}+1,i}^{g \rightarrow g'} \phi_l^g(r) + \int_V dV \int_{4\pi} d\hat{\Omega} \Gamma^{*g}(r, \hat{\Omega}) N_i \sigma_{s,\text{ISCT}+1,i}^{g \rightarrow g'} \psi^g(r, \hat{\Omega}). \quad (10)$$

The first term on the right side of Eq. (10) appears because of Eq. (4); the second term appears because of Eq. (3). Comparing Eqs. (1) and (2) with Eqs. (3) and (4), when diagonal transport correction is used, the relative sensitivity of R to the scattering cross section $\sigma_{s,\text{ISCT}+1,i}^{g \rightarrow g'}$ is $\delta_{gg'} S_{R,\sigma_{s,\text{ISCT}+1,i}}^{g \rightarrow g'}$, or just the diagonal elements of the sensitivity matrix. Note that Γ_l^{*g} in the first term on the right side of Eq. (10) has the index g of the “from” group, not the g' of the “to” group normally associated with scattering [as in, for example, the first term on the right side of Eq. (7)]. This is because only the self-scattering cross section is corrected [Eq. (4)]. The previous version of this report⁵ missed this point and had the wrong index.

When diagonal transport correction is used, the relative sensitivity S_{R,N_i}^g in group g of R to the density of isotope i is

$$S_{R,N_i}^g = S_{R,\nu_i}^g + S_{R,\sigma_{t,i}}^g + S_{R,\sigma_{s,i}}^g + S_{R,\sigma_{s,ISCT+1,i}}^{g \rightarrow g}, \quad (11)$$

and when BHS transport correction is used, the relative sensitivity S_{R,N_i}^g in group g of R to the density of isotope i is

$$S_{R,N_i}^g = S_{R,\nu_i}^g + S_{R,\sigma_{t,i}}^g + S_{R,\sigma_{s,i}}^g + \sum_{g'=1}^G S_{R,\sigma_{s,ISCT+1,i}}^{g \rightarrow g'}. \quad (12)$$

From Eq. (5), when Cesàro transport correction is used, then the modified relative sensitivity $\tilde{S}_{R,\sigma_{s,i}}^{g \rightarrow g'}$ of R to the scattering cross section $\sigma_{s,l,i}^{g \rightarrow g'}$ of isotope i for expansion order l from energy group g to g' is

$$\begin{aligned} \tilde{S}_{R,\sigma_{s,i}}^{g \rightarrow g'} &= \frac{(ISCT+2-l)(ISCT+1-l)}{(ISCT+2)(ISCT+1)} \int_V dV \Gamma_l^{*g'}(r) N_i (2l+1) \sigma_{s,l,i}^{g \rightarrow g'} \phi_l^g(r) \\ &\quad - \delta_{l0} \int_V dV \int_{4\pi} d\hat{\Omega} \Gamma^{*g}(r, \hat{\Omega}) N_i \sigma_{s,0,i}^{g \rightarrow g'} \psi^g(r, \hat{\Omega}). \end{aligned} \quad (13)$$

Likewise, the modified relative sensitivity to total scattering out of group g is

$$\tilde{S}_{R,\sigma_{s,i}}^g = \sum_{l=0}^L \frac{(ISCT+2-l)(ISCT+1-l)}{(ISCT+2)(ISCT+1)} \int_V dV \sum_{g'=1}^G \Gamma_l^{*g'}(r) N_i (2l+1) \sigma_{s,l,i}^{g \rightarrow g'} \phi_l^g(r). \quad (14)$$

Thus, when Cesàro transport correction is used, the relative sensitivity S_{R,N_i}^g in group g of R to the density of isotope i is

$$S_{R,N_i}^g = S_{R,\nu_i}^g + S_{R,\sigma_{t,i}}^g + \tilde{S}_{R,\sigma_{s,i}}^g. \quad (15)$$

IV. Implementation

SENSMG normally reads cross sections from PARTISN output files (`macrxs` and `sxnedt`), where scattering cross sections are available only up to order $ISCT$. Thus, for diagonal and BHS transport corrections, some coding had to be written to read scattering cross sections of order $ISCT+1$. It was decided to not use the Nuclear Data Interface (NDI) but instead to read the cross-section files directly and collapse the cross sections. The scattering cross sections of order $ISCT+1$ are also read if the Kynea3 cross section library,⁶ a bxslib-formatted file,¹ is used. If a particular nuclide does not have scattering of order $ISCT+1$, then SENSMG issues a warning that transport correction is not available for that nuclide (for diagonal or BHS transport corrections).

Reading the scattering cross sections for each isotope was not difficult, but collapsing them to the right group structure was a little tricky. With help from Thomas Saller (CCS-2) and Mark Gray (XCP-8), I figured out how the NDI collapses data. The spectrum weighting function f_i^g for isotope i in coarse groups $g = 1, \dots, G$ is collapsed from the spectrum weighting function $f_i^{g_f}$ for isotope i in fine groups $g_f = 1, \dots, G_f$ using

$$f_i^g = \sum_{g_f \in g} f_i^{g_f}, \quad (16)$$

where $g_f \in g$ indicates the fine groups g_f contained within coarse group g . In Eq. (16), fine-group energies larger than the largest coarse-group energy and fine-group energies smaller than the smallest

coarse-group energy are ignored. (The collapsed spectrum weighting function f_i^g is also needed for computing the sensitivity of the induced-fission isotopic χ vector.^{3,7}) The scattering cross section $\sigma_{s,l,i}^{g \rightarrow g'}$ for isotope i of expansion order l from group g to group g' is collapsed using

$$\sigma_{s,l,i}^{g \rightarrow g'} = \begin{cases} \frac{1}{f_i^g} \sum_{g' \in \{g', g'_{f-}\}} \sum_{g_f \in g} \sigma_{s,l,i}^{g_f \rightarrow g'} f_i^{g_f}, & g' = 1 \\ \frac{1}{f_i^g} \sum_{g_f \in g'} \sum_{g_f \in g} \sigma_{s,l,i}^{g_f \rightarrow g'} f_i^{g_f}, & 1 < g' < G \\ \frac{1}{f_i^g} \sum_{g' \in \{g', g'_{f+}\}} \sum_{g_f \in g} \sigma_{s,l,i}^{g_f \rightarrow g'} f_i^{g_f}, & g' = G, \end{cases} \quad (17)$$

where g'_{f-} indicates all fine groups above the largest coarse-group boundary and g'_{f+} indicates all fine groups below the smallest coarse-group boundary. The third line on the right side of Eq. (17) indicates that scattering into the bottom coarse group includes scattering into all fine groups below the lowest coarse group boundary, not just the fine groups within the lowest coarse group. The first line indicates that scattering into the top coarse group includes scattering into all fine groups above the largest coarse group boundary, not just the fine groups within the largest coarse group. This procedure preserves neutrons, but it distorts the energy spectrum.

Equations (16) and (17) assume that the $G + 1$ coarse-group boundaries are coincident with boundaries in the fine-group structure. The fine-group boundaries are in the cross section tables and the coarse-group boundaries are in SENSMSG data files, having been obtained from the group structures listed at <https://xweb.lanl.gov/projects/data/nuclear/ndi_data/transport/group_structure.html>. The energy-group boundaries on the web do not always match exactly the energy-group boundaries in the NDI cross section files. Therefore, in SENSMSG the requirement is that the energy-group boundaries match within a certain tolerance. Presently that tolerance, parameter `tol` in subroutine `rdnditable`, is 0.001%.

For diagonal and BHS transport corrections, the macroscopic total and self-scatter cross sections are modified [Eqs. (1) through (4)] for the transport, but the sensitivity of R to the microscopic total and self-scatter cross sections is unaffected by the transport correction, except indirectly through the forward and adjoint fluxes. In other words, Eqs. (6) and (7) are still used for $S_{R,\sigma_{t,i}}^g$ and $S_{R,\sigma_{s,i}}^{g \rightarrow g'}$. The output of these sensitivities is unaffected by the transport correction.

For the BHS transport correction, Eq. (10) is used for $S_{R,\sigma_{s,i}}^{g \rightarrow g'}$. The sensitivity matrix is printed immediately after the sensitivity matrices $S_{R,\sigma_{s,i}}^{g \rightarrow g'}, l = 1, \dots, \text{ISCT}$. No group sums of $S_{R,\sigma_{s,i}}^{g \rightarrow g'}$ are printed. All of this is also true for the diagonal transport correction except that the output matrix is diagonal, $\delta_{gg'} S_{R,\sigma_{s,i}}^{g \rightarrow g'}$.

For diagonal and BHS transport corrections, a new term is added to the isotope and material density sensitivities, the last term on the right side of Eqs. (11) and (12). An analogous term is added to the interface- and boundary-location derivatives and included in the output.

For the Cesàro transport correction, the total cross section is unaffected and Eq. (6) is used for $S_{R,\sigma_{t,i}}^g$. However, a new equation, Eq. (13), is used for the sensitivity of R to the microscopic scattering cross sections. In-scattering, self-scattering, and out-scattering group sums of all orders $l > 0$ are affected, as are the sensitivity matrices for all orders $l > 0$.

For the Cesàro transport correction, the same equation is used for isotope and material density sensitivities as when no transport correction is applied, Eq. (15), but the scattering sensitivity is modified, Eq. (14). An analogous equation is used for the interface- and boundary-location derivatives.

For cylinders in SENSMSG, the second term on the right side of Eq. (10) is approximated using a moments expansion,^{2,3}

$$\int_V dV \int_{4\pi} d\hat{\Omega} \Gamma_l^{*g}(r, \hat{\Omega}) N_i \sigma_{s,\text{ISCT}+1,i}^{g \rightarrow g'} \psi_l^g(r, \hat{\Omega}) \approx \int_V dV \sum_{l=0}^L (2l+1) \Gamma_l^{*g}(r) N_i \sigma_{s,\text{ISCT}+1,i}^{g \rightarrow g'} \psi_l^g(r). \quad (18)$$

This approximation is used in order to save memory. Unfortunately, this means that $S_{R,\sigma_{s,\text{ISCT}+1,i}}^{g \rightarrow g'}$ is zero for cylinders—the two addends on the right side of Eq. (10) cancel. The moments-expansion approximation can be lifted for some cylindrical problems, but the source code has to be modified.

When SENSMSG prints cross sections (with the `-wrxsecs` option³), it prints original, unmodified cross sections. For diagonal and BHS transport corrections, SENSMSG prints for each material and nuclide the $\sigma_{s,\text{ISCT}+1,i}^{g \rightarrow g'}$ cross sections, since they affect the transport. PARTISN should be so thoughtful.

V. Analytic Verification

The analytic S_2 one-group “rod” problem of Refs. 8 and 9 was used to verify the equations and implementation. The problem used isotropic scattering with diagonal transport correction (diagonal and BHS transport corrections are equivalent for this one-group problem). In the derivation of the analytic solution, Σ_t and Σ_s are replaced with $\Sigma_t - \Sigma_{s,1}$ and $\Sigma_s - \Sigma_{s,1}$, respectively, everywhere (Σ_s is the isotropic scattering cross section). The quantity $(\Sigma_t - \frac{1}{2}\Sigma_s - \frac{1}{2}\chi\nu\Sigma_f)$ becomes $(\Sigma_t - \frac{1}{2}\Sigma_s - \frac{1}{2}\Sigma_{s,1} - \frac{1}{2}\chi\nu\Sigma_f)$. The quantity $(\Sigma_s + \chi\nu\Sigma_f)$ becomes $(\Sigma_s - \Sigma_{s,1} + \chi\nu\Sigma_f)$. The quantity $(\Sigma_t - \Sigma_s - \chi\nu\Sigma_f)$ is unchanged. The derivatives of $(\Sigma_t - \Sigma_{s,1})$, $(\Sigma_t - \frac{1}{2}\Sigma_s - \frac{1}{2}\Sigma_{s,1} - \frac{1}{2}\chi\nu\Sigma_f)$, and $(\Sigma_s - \Sigma_{s,1} + \chi\nu\Sigma_f)$ with respect to the P_1 scattering cross section $\sigma_{s,1,X}$ of nuclide X are $-N_X$, $-\frac{1}{2}N_X$, and $-N_X$, respectively.

The relative sensitivities from SENSMSG of the count rate R_1 , the second moment R_2 , and the Feynman Y with respect to the P_1 scattering cross sections of Pu-239 and Pu-240 are compared to the analytic values in Tables I and II. The agreement is excellent.

Table I. Relative Sensitivities to $\sigma_{s,l,\text{Pu 239}}$.

Sensitivity	Analytic	SENSMG	Difference
$S_{R_1, \sigma_{s,l,\text{Pu 239}}}$	-2.910637E-01	-2.910637E-01	0.00001%
$S_{R_2, \sigma_{s,l,\text{Pu 239}}}$	-9.055435E-01	-9.055436E-01	-0.00001%
$S_{Y, \sigma_{s,l,\text{Pu 239}}}$	-6.144799E-01	-6.144799E-01	0.00000%

Table II. Relative Sensitivities to $\sigma_{s,l,\text{Pu 240}}$.

Sensitivity	Analytic	SENSMG	Difference
$S_{R_1, \sigma_{s,l,\text{Pu 240}}}$	-1.159303E-02	-1.159303E-02	-0.00003%
$S_{R_2, \sigma_{s,l,\text{Pu 240}}}$	-3.606770E-02	-3.606770E-02	0.00000%
$S_{Y, \sigma_{s,l,\text{Pu 240}}}$	-2.447466E-02	-2.447467E-02	-0.00002%

VI. Multiregion, Multigroup Sphere

This test problem used the one-dimensional spherical Flattop-Pu critical benchmark.¹⁰ Dimensions, densities, and material compositions are given in Table III. The full SENSMSG input file is listed in the appendix. The response was k_{eff} .

Table III. Flattop-Pu Model.

Material	Outer Radius (cm)	Density (g/cm ³)	Isotope	Weight Fraction
Plutonium	4.5332	15.53	Pu-239	9.38001E-01
			Pu-240	4.79988E-02
			Pu-241	2.99996E-03
			Ga-69	6.53652E-03
			Ga-71	4.46355E-03
Natural Uranium	24.142	19.00	U-234	5.40778E-05
			U-235	7.10966E-03
			U-238	9.92836E-01

An angular quadrature of S_{32} and fine mesh spacing of 0.005 cm were used. MENDF71X cross sections collapsed to 30 groups were used. PARTISN version 8.32.52 was used. Prior PARTISN versions, including the present RSICC version (8.29.32), have a bug that affects adjoint calculations that use the BHS transport correction. As a result, adjoint results are not correct and sensitivities computed using them are also not correct. The bug was fixed in version 8.32.52.¹¹

This problem was run with various scattering expansion orders and each of the transport corrections (including none). The k_{eff} multiplication factors are compared in Table IV. The benchmark k_{eff} is¹⁰ 1.00000 ± 0.00300 (four digits are given in Ref. 10; five are given here for consistency with Table IV).

Table IV. Flattop-Pu k_{eff} as a Function of Transport Correction and Scattering Order.

TRCOR	ISCT	k_{eff}	TRCOR	ISCT	k_{eff}
No	0	1.1483219	BHS	0	1.0122982
	1	0.97860362		1	0.99970394
	2	1.0071033		2	1.0013844
	3	0.99932409		3	1.0008393
	4	1.0014397		4	1.0014397
Diagonal	0	1.0129424	Cesàro	0	1.1483219
	1	0.99972843		1	1.0973197
	2	1.0013906		2	1.0734168
	3	1.0008348		3	1.0589500
	4	1.0014397		4	1.0493153

Conclusions from Table IV are:

1. The Cesàro transport correction is wildly inaccurate for this problem. Even at the highest scattering expansion order, k_{eff} is far outside the uncertainty range of the benchmark. The PARTISN manual does caution the user regarding the use of the Cesàro correction (Ref. 1, p. 3-28). A stronger warning has been put into the SENSIMG manual and the SENSIMG output.
2. The diagonal and BHS transport corrections have about the same accuracy for this problem.
3. For small scattering expansion orders (0, 1, and 2), the diagonal and BHS transport corrections are more accurate than no transport correction. For a scattering expansion order of 3, the accuracy is approximately the same.
4. For a scattering expansion order of 4, k_{eff} s using no correction, diagonal correction, and BHS correction are equal. This is because 4 is the limit of the scattering expansion in the data—i.e., there is no $\Sigma_{s,ISCT+1}^{g \rightarrow g'}$ to use in Eqs. (1) through (4)—so PARTISN cannot apply the requested transport correction. It writes the message “isct too large for transport correction” and solves the problem with no correction. SENSIMG writes the message “no transport correction for isotope [isotope specified]”.
5. As the PARTISN manual states, there is no Cesàro transport correction for isotropic scattering ($l = 0$). That is why the Cesàro result is the same as the no-correction result for ISCT = 0.
6. The conventional wisdom that P_3 scattering is more accurate than P_4 is true for this problem using these nuclear data.

The adjoint-based (SENSMG) relative sensitivity of each of the material densities, computed without accounting for the effect of the transport corrections on the sensitivities, was compared with a central-difference estimate for various scattering expansion orders and each of the transport corrections (including none). For the central differences, the plutonium mass density was perturbed $\pm 0.1\%$ and (separately) the uranium mass density was perturbed $\pm 1\%$. Results are shown in Table V.

Conclusions from Table V are:

1. The SENS MG sensitivities compare very well with the central differences when there is no transport correction. This is a verification of the coding, not the math; the adjoint based sensitivities are exact.
2. For small scattering expansion orders (0, 1, and 2), there are large differences between the uncorrected SENS MG sensitivities and the central differences. This is because the uncorrected SENS MG sensitivities are inconsistent with the transport calculations, as discussed in Sec. II. They do not account for the transport corrections. For larger scattering expansion orders (3 and 4), the differences are smaller, except for the Cesàro correction.

The corrected adjoint-based (SENSMG) relative sensitivity of each of the material densities, which account for the effect of the transport corrections on the sensitivities, was also compared with the central-difference estimates. Results are shown in Table VI. The conclusion from Table VI is that the development and implementation of the equations that account for the effect of the transport corrections on the sensitivities is verified.

Table V is presented for information only. It is not a user option to turn off the correct accounting for any transport correction. SENS MG automatically accounts for the transport correction in the sensitivity calculations.

Table V. Uncorrected Relative Sensitivity to Material Density (%/%).

TRCOR	ISCT	Plutonium			Natural Uranium		
		SENSMG	CD	Diff.	SENSMG	CD	Diff.
No	0	6.52164E-01	6.52169E-01	-0.001%	2.19750E-01	2.19594E-01	0.071%
	1	6.83858E-01	6.83852E-01	0.001%	2.36938E-01	2.36684E-01	0.108%
	2	6.76182E-01	6.76147E-01	0.005%	2.18264E-01	2.18066E-01	0.091%
	3	6.78344E-01	6.78333E-01	0.002%	2.27833E-01	2.27629E-01	0.089%
	4	6.77880E-01	6.77425E-01	0.067%	2.23962E-01	2.23740E-01	0.099%
Diagonal	0	7.15760E-01	6.75112E-01	6.021%	3.26025E-01	2.19820E-01	48.315%
	1	6.76413E-01	6.78349E-01	-0.285%	2.03836E-01	2.25920E-01	-9.775%
	2	6.77858E-01	6.77857E-01	0.000%	2.30401E-01	2.24147E-01	2.790%
	3	6.77992E-01	6.78034E-01	-0.006%	2.23733E-01	2.25079E-01	-0.598%
	4	6.77880E-01	6.77425E-01	0.067%	2.23962E-01	2.23740E-01	0.099%
BHS	0	7.16107E-01	6.75196E-01	6.059%	3.26634E-01	2.19807E-01	48.600%
	1	6.76418E-01	6.78441E-01	-0.298%	2.03884E-01	2.25960E-01	-9.770%
	2	6.77860E-01	6.77862E-01	0.000%	2.30413E-01	2.24197E-01	2.773%
	3	6.77991E-01	6.78031E-01	-0.006%	2.23721E-01	2.25075E-01	-0.602%
	4	6.77880E-01	6.77425E-01	0.067%	2.23962E-01	2.23740E-01	0.099%
Cesàro	0	6.52164E-01	6.52126E-01	0.006%	2.19750E-01	2.19594E-01	0.071%
	1	6.37926E-01	6.62432E-01	-3.699%	1.53200E-01	2.25818E-01	-32.158%
	2	6.48376E-01	6.66563E-01	-2.728%	1.83393E-01	2.26473E-01	-19.022%
	3	6.54086E-01	6.69106E-01	-2.245%	1.88015E-01	2.26739E-01	-17.079%
	4	6.57946E-01	6.70580E-01	-1.884%	1.94819E-01	2.26734E-01	-14.076%

Table VI. Corrected Relative Sensitivity to Material Density (%/%).

TRCOR	ISCT	Plutonium			Natural Uranium		
		SENSMG	CD	Diff.	SENSMG	CD	Diff.
Diagonal	0	6.75196E-01	6.75112E-01	0.012%	2.20012E-01	2.19820E-01	0.088%
	1	6.78342E-01	6.78349E-01	-0.001%	2.26104E-01	2.25920E-01	0.081%
	2	6.77866E-01	6.77857E-01	0.001%	2.24356E-01	2.24147E-01	0.093%
	3	6.77998E-01	6.78034E-01	-0.005%	2.25291E-01	2.25079E-01	0.094%
	4	6.77880E-01	6.77425E-01	0.067%	2.23962E-01	2.23740E-01	0.099%
BHS	0	6.75151E-01	6.75196E-01	-0.007%	2.19998E-01	2.19807E-01	0.087%
	1	6.78344E-01	6.78441E-01	-0.014%	2.26135E-01	2.25960E-01	0.077%
	2	6.77868E-01	6.77862E-01	0.001%	2.24361E-01	2.24197E-01	0.073%
	3	6.77997E-01	6.78031E-01	-0.005%	2.25283E-01	2.25075E-01	0.093%
	4	6.77880E-01	6.77425E-01	0.067%	2.23962E-01	2.23740E-01	0.099%
Cesàro	0	6.52164E-01	6.52126E-01	0.006%	2.19750E-01	2.19594E-01	0.071%
	1	6.62417E-01	6.62432E-01	-0.002%	2.25993E-01	2.25818E-01	0.077%
	2	6.66583E-01	6.66563E-01	0.003%	2.26669E-01	2.26473E-01	0.087%
	3	6.69004E-01	6.69106E-01	-0.015%	2.26946E-01	2.26739E-01	0.091%
	4	6.70572E-01	6.70580E-01	-0.001%	2.26931E-01	2.26734E-01	0.087%

VII. Summary and Future Work

This report documents updates that have been made to SENSMSG to account for the effect of diagonal, BHS, and Cesàro transport corrections (all of the transport corrections available in PARTISN) on the calculated sensitivities. For diagonal and BHS transport corrections, the sensitivities of the response to the order ISCT + 1 group-to-group scattering cross sections are printed. For cylindrical geometries in SENSMSG, a moments expansion approximation means that the sensitivities of the response to the order ISCT + 1 group-to-group scattering cross sections are incorrectly reported to be zero.

This report also discusses how the NDI collapses the weight function and the scattering cross sections, because SENSMSG now does that too. SENSMSG collapses the weight functions in order to correctly compute the sensitivity of a response to the induced-fission χ vector.^{3,7} SENSMSG collapses the ISCT + 1 scattering cross sections in order to handle diagonal or BHS transport corrections. When the diagonal or BHS transport correction is used and cross sections are printed using the “-wrxsecs yes” option, the order ISCT + 1 group-to-group scattering cross sections are printed.

This report also demonstrates that Cesàro transport correction should be used with extreme caution, and it should not be used at all for fast critical systems such as the Flattop-Pu benchmark used in this report. SENSMSG prints a strong warning if Cesàro correction is used, but it is allowed.

Acknowledgments

This work was funded by the ASC program, Primary Validation & Verification project, at LANL.

References

1. R. E. Alcouffe, R. S. Baker, J. A. Dahl, E. J. Davis, N. H. Hart, M. I. Ortega, T. G. Saller, S. A. Turner, R. C. Ward, and R. J. Zerr, “PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System,” Los Alamos National Laboratory report LA-UR-17-29704 (Revised September 2020).
2. Jeffrey A. Favorite, “SENSMSG: First-Order Sensitivities of Neutron Reaction Rates, Reaction-Rate Ratios, Leakage, k_{eff} , and α Using PARTISN,” *Nuclear Science and Engineering*, **192**, 1, 80–114 (2018); <https://doi.org/10.1080/00295639.2018.1471296>.
3. Jeffrey A. Favorite, “(U) SENSMSG: First-Order Sensitivities of Neutron Reaction Rates, Reaction-Rate Ratios, Leakage, k_{eff} , α , and Subcritical Multiplication Using PARTISN,” XCP-3:19-022(U), Los Alamos National Laboratory report LA-UR-19-26249, Rev. 1 (September 19, 2019).
4. G. I. Bell, G. E. Hansen, and H. A. Sandmeier, “Multitable Treatments of Anisotropic Scattering in S_N Multigroup Transport Calculations,” *Nuclear Science and Engineering*, **28**, 3, 376–383 (1967); <https://doi.org/10.13182/NSE67-2>.
5. Jeffrey A. Favorite, “(U) Transport Corrections Implemented in SENSMSG,” XCP-3:19-026(U), Los Alamos National Laboratory report LA-UR-19-26249, Rev. 0 (August 20, 2019).

6. E. S. Varley and J. Mattingly, "Rapid Feynman-Y Synthesis: Kynea3 Cross-Section Library Development," *Transactions of the American Nuclear Society*, **98**, 575–576 (2008).
7. Jeffrey A. Favorite, "(U) Differences in the Use of Isotopic χ Vectors Demonstrated with an Analytic k_{∞} Problem (And Verification of SENSMSG and MCNP6's KSEN)," XCP-3:19-019(U), Los Alamos National Laboratory report LA-UR-19-24780 (May 22, 2019).
8. Jeffrey A. Favorite, "Analytic One-Group S_2 Slab Problem with Isotropic Scattering and Fission Applied to Leakage and Neutron Multiplicity Sensitivity," *Transactions of the American Nuclear Society*, **121**, 929–932 (2019).
9. Jeffrey A. Favorite, "(U) Analytic One-Group S_2 Slab Problem with Isotropic Scattering and Fission Applied to Leakage and Neutron Multiplicity Sensitivity," XCP-3:19-018(U), Los Alamos National Laboratory report LA-UR-19-24544 (May 16, 2019).
10. R. W. Brewer, T. P. McLaughlin, and Virginia Dean, "Plutonium Sphere Reflected by Normal Uranium Using Flattop," *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, PU-MET-FAST-006, Revision 1, Nuclear Energy Agency, Organization for Economic Co-Operation and Development (December 2016).
11. PARTISN 8.32 release notes (September 2020).

JAF:jaf

Distribution:

J. T. Goorley, XCP-7, MS A143, jgoorley@lanl.gov
M. C. White, P-27, MS H805, morgan@lanl.gov
R. S. Baker, CCS-2, MS D409, rsb@lanl.gov
J. A. Dahl, CCS-2, MS D409, dahl@lanl.gov
E. J. Davis, CCS-2, MS D409, ejdavis@lanl.gov
N. H. Hart, CCS-2, MS D409, nhhart@lanl.gov
M. I. Ortega, CCS-2, MS D413, mortega@lanl.gov
T. G. Saller, CCS-2, MS D409, tgsaller@lanl.gov
R. J. Zerr, CCS-2, MS D409, rzerr@lanl.gov
S. D. Ramsey, XTD-NTA, MS T082, ramsey@lanl.gov
C. D. Ahrens, XTD-PRI, MS T086, cdahrens@lanl.gov
E. F. Shores, XTD-SS, MS T082, eshores@lanl.gov
R. C. Little, XCP-DO, MS F663, rcl@lanl.gov
A. R. Clark, XCP-5, MS P365, arclark@lanl.gov
J. L. Conlin, XCP-5, MS F663, jlconlin@lanl.gov
W. Haeck, XCP-5, MS P365, wim@lanl.gov
D. K. Parsons, XCP-5, MS F663, dkp@lanl.gov
P. Talou, XCP-5, MS F644, talou@lanl.gov
J. L. Alwin, XCP-7, MS A143, jalwin@lanl.gov
J. A. Favorite, XCP-7, MS F663, fave@lanl.gov
National Security Research Center, nsrc-cataloging@lanl.gov
XCP-7 File

APPENDIX A INPUT FILES

SENSMG INPUT FILE FOR THE PROBLEM OF SEC. V

```
two-isotope slab
slab feyny
mendf71x
1 / no of materials
1 94239 -0.96 94240 -0.04 /
-14.00 / densities
1 / no of shells
0. 4. /
1 / material nos
0 / number of edit points
0 / number of reaction-rate ratios
0 / number of njoy reactions
```

As in Refs. 8 and 9, the two-isotope slab was run with a mesh spacing of 0.0005 cm, which was achieved by modifying the SENSMSG source code.

SENSMG INPUT FILE FOR THE PROBLEM OF SEC. VI

```
Pu-Flattop (PU-MET-FAST-006)
keff sphere
mendf71x
2 / no of materials
1 94239 -9.38001E-01 94240 -4.79988E-02 94241 -2.99996E-03 31069 -6.53652E-
03 31071 -4.46355E-03 / Pu-alloy
2 92234 -5.40778E-05 92235 -7.10966E-03 92238 -9.92836E-01 / Flattop natural
U
-15.53 -19.00 / densities
3 / no of shells
0.5 4.5332 24.142 / outer radii
1 1 2 / material nos
0 / number of edit points
0 / number of reaction-rate ratios
0 / number of njoy reactions
```

The following C-SHELL script was used to run the Pu-Flatop input file:

```
#!/bin/csh
setenv NDI_GENDIR_PATH
/usr/projects/data/nuclear/ndi/2.1.3/share/gendir.all
setenv SENS_PARTISN /usr/projects/lindet/releases/rel8_32/8_32_52/cts1-
intel-19.0.4-openmpi-2.1.2/partisn
set SENSMG="/usr/projects/transportapps/users/fave/sensmg/bin/sensmg.py"

echo STARTING RUN: `date "+ %D %H:%M:%S"`
set inp="B"
foreach trcor ( no diag bhs cesaro )
    foreach isct ( 0 1 2 3 4 5 )
        ${SENSMG} -i ${inp} -isn 32 -ngroup 30 -np 24 -isct ${isct} -trcor
${trcor}
        set ext = ${isct}.${trcor}
        foreach o ( for adj xs1 )
            if ( -e ${inp}.${o}.${ext} ) then
                rm -rf ${inp}.${o}.${ext}
            endif
        end
        foreach o ( sens_k_x sens_k_r sensmg.log for adj xs1 )
            if ( -e ${o} ) then
                mv ${o} ${inp}.${o}.${ext}
            endif
        end
    end
end
echo FINISHED RUN: `date "+ %D %H:%M:%S"`
```